optimization, designed to deal with challenges of costly, noisy computations. Simultaneously, simulated exploration of potential alternative sources of experimental data for monitoring bulk assembly (e.g, non-covalent mass spectrometry) suggest that other feasible technologies providing richer data on assembly progress can more precisely pin down true parameters and assembly pathways. Advancing such simulation-based data fitting methods provides a general technology for greatly enhancing our ability to learn fine-scale details of complex assembly processes from experimental data, a strategy with potential application to developing accurate quantitative models of numerous other assembly systems found through biology.

2373-Pos Board B510
A Computational Model of Cell-Generated Traction Forces and Fibronectin Assembly
Seth H. Weinberg[1], Lewis E. Scott[2], Devin B. Mair[2], Christopher A. Lemmon[2].
[1]Virginia Modeling, Analysis and Simulation Center, Old Dominion University, Suffolk, VA, USA, [2]Biomedical Engineering, Virginia Commonwealth University, Richmond, VA, USA.
The extracellular matrix (ECM) is an assembly of proteins that surround cells, and serves as the cell substrate in vivo. A primary component of newly synthesized ECM is the fibronectin (FN). Despite many years of research, the mechanism of FN assembly is still not completely understood. While it is recognized that FN assembly requires application of traction force to expose a buried FN-FN binding site, such a site has never been elucidated. We hypothesize that assembly of fibronectin (FN) fibrils is a complex event: each of the 15 Type III domains in FN is made up of a sandwich of 7 beta strands; when relaxed, the Type III domains are folded such that the beta strands are twisted, blocking the non-specific binding of other proteins. Application of force straightens these beta-strands, allowing for binding of other FNs via a beta-strand addition mechanism. This suggests that all 15 domains are capable of binding FN molecules in a growing fibril. To investigate this hypothesis, we present a mechanistic computational model of cell/FN/substrate biomechanical interactions, which accounts for the unique, nonlinear mechanical properties of each domain and the stochastic binding between molecular clutches and the moving actin bundle. Monte Carlo simulations predict that increasing substrate stiffness leads to longer and thicker fibrils. Additionally, the model demonstrates complex time-dependent dynamics governing the size of the growing fibril, the domains' stiffness, and traction forces; that is, at low force, a small subset of domains open, allowing for minimal fibril assembly, while large forces unfold a considerable fraction of domains and create large, thick fibrils. Simulation outputs are compared to experimental data in which traction force, FN assembly, and domain opening are quantified using microfabricated pillar arrays and cysteine-labeling of recombinant FNs with introduced buried cysteines.

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Numerical Modeling of Lipid Biosynthesis in Microalgae
Nicole J. Carbonaro, May M. Li, Matthew W. Sweeney, Ian F. Thorpe.
Chemistry and Biochemistry, University of Maryland, Baltimore County, Catonsville, MD, USA.
A worldwide effort to find renewable alternatives to fossil fuels is underway. Potential sources of renewable fuel include microalgae. Under certain conditions, these organisms produce large amounts of triacylglycerides (TAGs), lipids that can be converted to biodiesel. However, the lipid biosynthetic pathway of microalgae is not fully understood. To better understand the conditions that govern lipid production in microalgae, we employ theoretical and computational methods to understand the topology, flux and regulatory properties of the metabolic pathway involved in TAG biosynthesis in microalgae. In particular, we seek to understand the differences that lead to altered TAG production in different microalgal species. We compare a species that naturally generates large amounts of TAG under stress conditions with a species that produces comparatively much less TAG under similar conditions. Predictions from the model will be validated by comparison with in vitro and in vivo experiments. By understanding more about lipid production in microalgae we hope to guide rational genetic engineering approaches to increase oil production in these organisms. We anticipate that these studies will ultimately provide insights into lipid biosynthesis for a wide range of other organisms.

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Robust Elastic Network Model: Precise Prediction of Atomic Fluctuations in Protein Crystal Structures
Min Hyeok Kim, Byung Ho Lee, Moon Ki Kim.
Sungkwunkwan university, Sowon, Korea, Republic of.
Elastic network model (ENM) based normal mode analysis has become popular as its capability and suitability for the study of protein dynamics. However, the existing ENMs often fail to reproduce the experimentally observed B-factor (i.e., atomic fluctuation) because of oversimplification of their force-fields. In this work, we have proposed a robust ENM (RENM) in which, for reflecting inter-connections accused from surrounding molecules in a unit cell, symmetric constraints based on crystal space group are applied to the representative single molecule as well as its intra-connections are also represented by using lumped masses and specific spring constants depending on the types of amino acids and chemical bonds, respectively. More than 500 protein structures are tested by RENM. Their results show better agreement with experimental B-factor without additional computation burden compared to those of traditional ENM. Moreover, the global spring constant is quantitatively determined as a function of temperature at 100K and 290K, which enables us to compute directly atomic fluctuations and vibrational density of state without any fitting process. Thus, RENM is expected to play an important role in understanding protein dynamics based on its crystal structure information.

2376-Pos Board B513
Protein Translocation through an Electrically Tunable Membrane
Ining Amy Jou, Dmitriy V. Melnikov, **Maria Gracheva**.
Department of Physics, Clarkson University, Potsdam, NY, USA.
Understanding protein dynamics through an artificial nanopore has implications in many areas such as sensing and filtering. Collecting statistical information while tracking the movement of a full atomic protein model is computationally expensive since number of atoms ranges in the thousands. The need to represent protein with a computationally cost effective model is imperative, along with understanding its dynamics through the nanopore. In this work we studied the dynamics of the protein insulin placed near a nanopore of an electrically tunable semiconductor membrane. Using Brownian dynamics method we calculated the trajectory of the modeled protein in the electrolyte-membrane electrostatic potential. The time spent by the protein before a successful translocation and the translocation times were both analyzed. Our results indicate that the localized electric field within the nanopore affects the movement of the protein. Also, by comparing the results of the full atomic protein model with a coarse grained model and a single bead model, we evaluate which model best approximates the full atomic protein model.

2377-Pos Board B514
Traveling Wave Solutions to Reaction-Diffusion Equations based on the Lambert W Function
Brian W. Williams.
Department of Chemistry, Bucknell University, Lewisburg, PA, USA.
Non-linear partial differential equations of the ''reaction-diffusion'' arise in many areas of biological, chemical and physical science, including the Burgers-Huxley equation associated with nerve pulses. Solutions to these types of equations are often found in the form of traveling waves, which in one dimension propagate over the entire real axis between stable limits for non-negative time. The generalization of known non-linear model equations continues to remain of interest.
It is shown here that it is possible to find traveling wave solutions to a generalized group of reaction-diffusion equations of this type, based on a traveling wave which can be represented in terms of the Lambert W function. This approach begins by considering the first order differential equation exactly solved by the traveling wave, and then using an operator approach to construct a second order differential equation solvable in terms of this traveling wave. The second-order differential equation can then be compared to the original partial differential equation after a transformation of the variables.

2378-Pos Board B515
Quantitative Theory of Active Diffusion Trajectories by Instantaneous Diffusion Coefficient
Soya Shinkai, Yuichi Togashi.
RcMcD, Hiroshima University, Higashi-Hiroshima, Japan.
Owing to the development of single-particle tracking techniques, it is able to observe real-time diffusive motions of labelled tiny particles in living cells. To quantify the diffusion trajectories, the mean-squared displacement (MSD) analysis is common and conventional. The diffusion coefficient quantified by the analysis is a good barometer of the mobility. But, in terms of statistical physics, equilibrium and stationarity are assumed in the MSD analysis. Accordingly, the analysis depends on the statistical ensemble. When diffusive motions are driven by non-equilibrium and non-stationary fluctuations as the outcome of biological activity, such fluctuations are averaged and neglected in the MSD analysis. Such enhanced diffusive motion is called active diffusion. To understand the interaction among diffusive motion, biological activity, and environment in detail, we should develop a new diffusion analysis theory beyond the MSD analysis.
Hence, our subject is not an ensemble of diffusion trajectories, only individual ones. The MSD analysis is based on the hypothesis of a stationary stochastic